Automated Analysis of Phase Diagrams

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I. Motivation

Phase diagrams serve as a mapping of phase stability in the context of extrinsic variables such as chemical composition with respect to temperature and/or pressure and they are valuable tools for material scientists in their quest for discovery of new materials with desired properties. The geometrical characteristics of phase diagrams, including the shape of phase boundaries and positions of phase boundary junctions have fundamental thermodynamic origins. Hence they serve as a visual signature of the nature of thermochemical properties of alloys. The design of alloys for instance relies on inspection of many such documented phase diagrams and this is usually a manual process. Our objective is to develop an automated document recognition tool that can process large quantities of phase diagrams in order to support user queries which, in turn, facilitate the simultaneous screening of a large number of materials without loss of information.

Further, from the phase diagram images, we readily identify specific types of phase boundary junctions, known as ‘eutectic points’. We have used this test case to show that we can rapidly identify certain geometrical characteristics of a class of eutectic points known as ‘deep eutectics’, that could be potentially be the chemical foundation for amorphous alloys (also known as ‘metallic-glasses’).

For this paper, we randomly select a small subset of phase diagrams of binary metallic alloy systems where the X-axis is molar fraction percentage and the Y axis is temperature. The goal of our pilot study is to create a database, where given a temperature value and molar fraction percentage for a particular alloy, the database returns the phase of the alloy.

Although graphics analysis and understanding has been an active area of interest in the document analysis community, to the best of our knowledge, no prior work has tackled the problem of analyzing and understanding diagrams of interest to the material science community, such as phase diagrams. We are primarily interested in analyzing the structure of the graphic and interpreting the technical information latent in these diagrams. So, we not only attempt to understand elements of plots such as axis labels and legends, but we also process contours and text within the main graphic area to identify critical information of interest to materials science researchers, such as phase values for all points within contours, and semantically critical points of interest.

Phase diagrams need specific attention primarily because of the way the information is embedded into the diagram. The lines in a phase diagram are not of a continuously changing value like in a line plot, but instead represent a boundary. A phase diagram cannot be expressed by a simple table like most line plots, bar charts etc. Further, text could appear in different orientations and associating the text with phase regions (and sometimes vertical lines) is an added complexity that is non-trivial and essential to the final interpretation by material science domain experts. These characteristics underline the necessity for having a targeted approach to handling this particular class of diagrams.

II. Overview of our approach

From a document analysis perspective, a phase diagram can be seen to consist mainly of alphanumeric text, often with accompanying Greek characters, in vertical and horizontal orientations; bounded regions of uniform phase within the plot; descriptions of axes and numerical quantities along the axes. As can be seen in Figure 1, narrow and small phase regions, presence of arrows, text located very close to phase boundaries and different orientations pose steep challenges for automated analysis. The key steps in automated phase diagram analysis are listed below and will be elaborated in the sections that follow:

- detection and recognition of text used to label phases
- extraction of regions of uniform phases
- association of each phase region to appropriate labels (including detection of arrows)
- detection and recognition of Y-axis and X-axis quantities

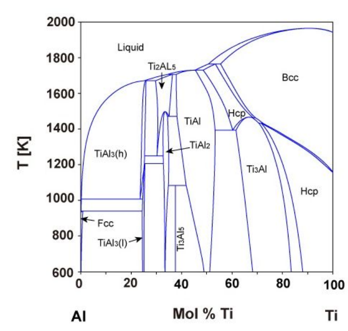

Fig. 1. Example of a challenging phase diagram.

Phase diagram images are obtained from the same source - Computational Phase Diagram Database [1] collected by

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National Institute of Material Sciences so that the phase labeling, plot and image styling are consistent. We gathered about 80 different phase diagrams of binary alloys consisting of a number of common transition metals and main group metals.

Each image is preprocessed and contours are extracted using the algorithm proposed by Suzuki and Abe [2]. We extract geometric and moments-based features from each contour and a gradient boosted tree-based classifier is trained to classify between phase contours and text contours with high accuracy.

After classification of contours into text and phase contours, we concentrate on grouping the text contours into words and recognizing the text, so that these word labels can then be mapped to the appropriate phase contours. We group the text contours which correspond to characters or groups of characters into vertical and horizontal words based on inter-character distances and empirical thresholds following which the text is recognized using the Tesseract library [3].

Arrows occur frequently in our dataset (seen in Figure 1) and need to be identified in order to accurately match text contours to corresponding phase contour. We use a Hough line detector to detect arrows. Collinear and/or overlapping line segments are merged and redundant sections are removed to yield the list of arrows in the image. For every arrow, we find the word region closest to the tail and the phase contour or vertical line closest to the head and these are stored as matched pairs.

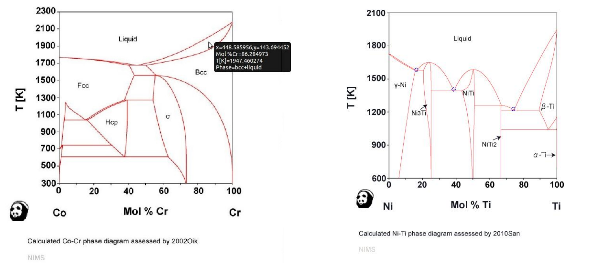
Once the text within the plot is grouped and recognized and the arrows in the image have been dealt with, we proceed to associate the rest of the text labels to the appropriate phase regions and boundary lines. Vertical words are mapped to the nearest unlabeled vertical line by measuring the perpendicular distance between the centroid of the word bounding box and the line. After this, we match phase regions to horizontal text labels by finding the text bounding boxes that are fully contained within the phase region. We resolve conflicts, if any, by giving priority to text labels whose centroid is closest to that of the phase region. Labels for unlabeled phase contours are inferred using standard rules.

Text on the axes is read and used to translate the image coordinates (x, y) to the physical coordinates $(mole fraction, temperature)$ and identify the metals in the plot. With this we will be able to query any required physical coordinate for any binary alloy, convert it to image coordinates and find the phase contour which contains this point and return the label assigned to the contour.

Aside from the phase information, we also detect 'eutectic points' (see Section I), which are point(s) in a phase diagram indicating the chemical composition and temperature corresponding to the lowest melting point of a mixture of components. These points serve as an important first order signature of alloy chemistries and are vital for design of 'metallic-glasses' which have a wide variety of applications. The eutectic points can be determined by analyzing the contour of the liquid phase for which both contour separation and accurate matching of label and region is critical. An example is seen in Figure 2 (b). Blue circles are used to mark the location of eutectic points.

III. Evaluation and Discussion

Fig. 2. Demo of our live phase query retrieval system for a signal query and detection of eutectic points. Best viewed in color.



(a) Demo of our live phase query retrieval system for a single phase query.

(b) Detection of eutectic points, shown in blue circles.

We report our accuracy of phase contour labeling for both cases - labels present within the phase diagram (94%) and labels that have to be inferred (88%) and the results show promise. Our contour extraction and text classification works well even for varied contour sizes and shapes. A small demo application constructed using our methods is shown in Figure 2 (a), where we display the transformed physical coordinates as well as the phase of the material at the cursor position. Given the importance of a digitized phase diagram database to the materials community at large, we believe that our efforts in this direction are worthwhile. In the future, we would like to create and release a comprehensive, high resolution database of phase diagrams, and work on a more general framework to interpret other types of phase diagrams and extend our work to support the detection and storage of other critical points that are important for design and manufacture of certain materials. Further, the materials domain is rich in graphs, figures and tables that contain valuable information, which when combined and collated into a large searchable, digital databases, would help the materials community in their quest to accelerate the discovery of newer and more exciting materials.

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